

A

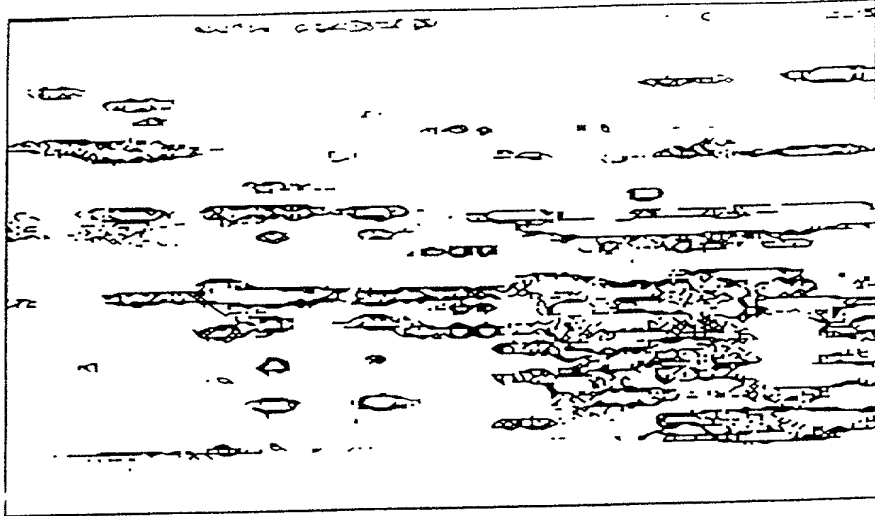
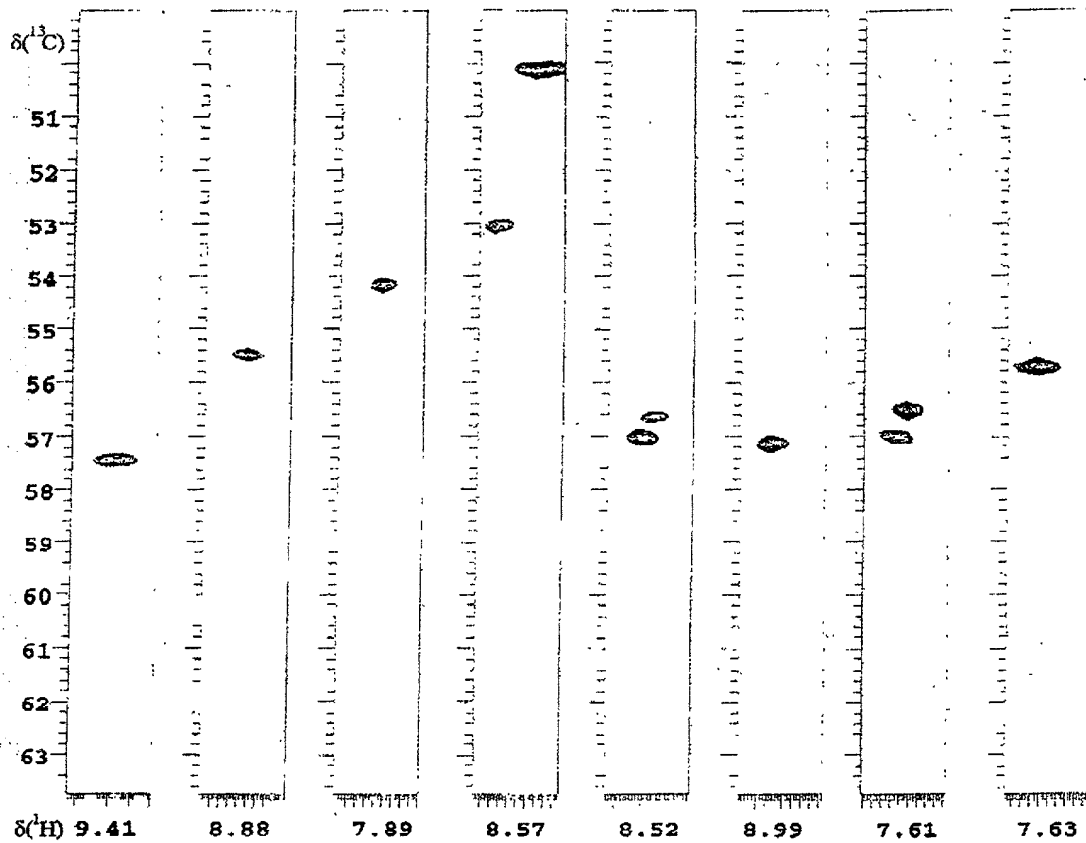
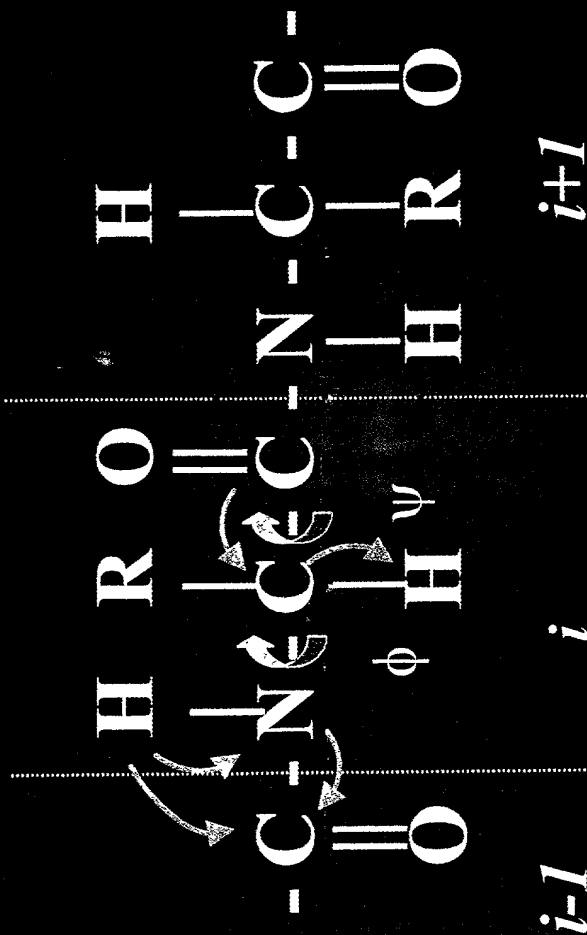


FIGURE 1B



Dipolar Couplings That Depend Only on $\phi(i)$ and $\psi(i)$



Search ϕ and ψ Until Measured Couplings = Theoretical Couplings

Packing Secondary Structural Elements

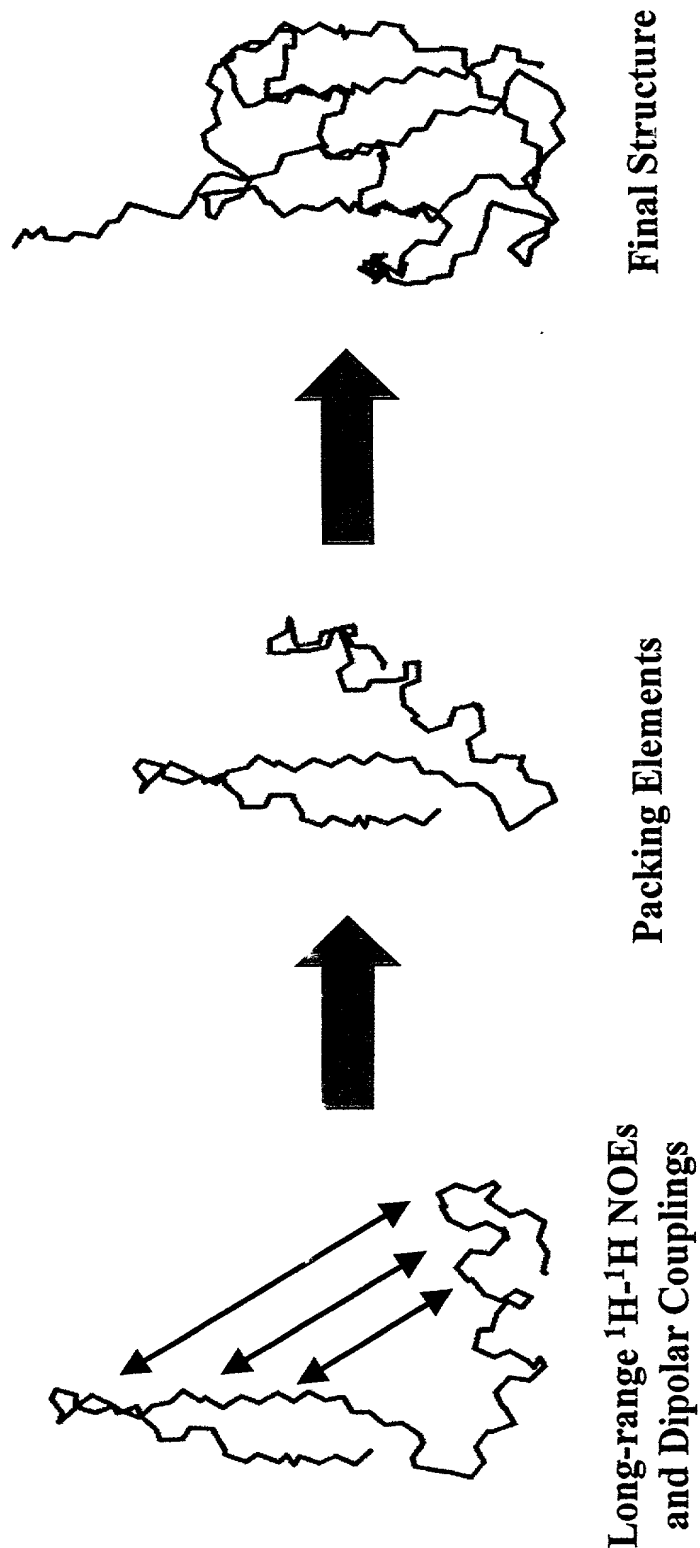
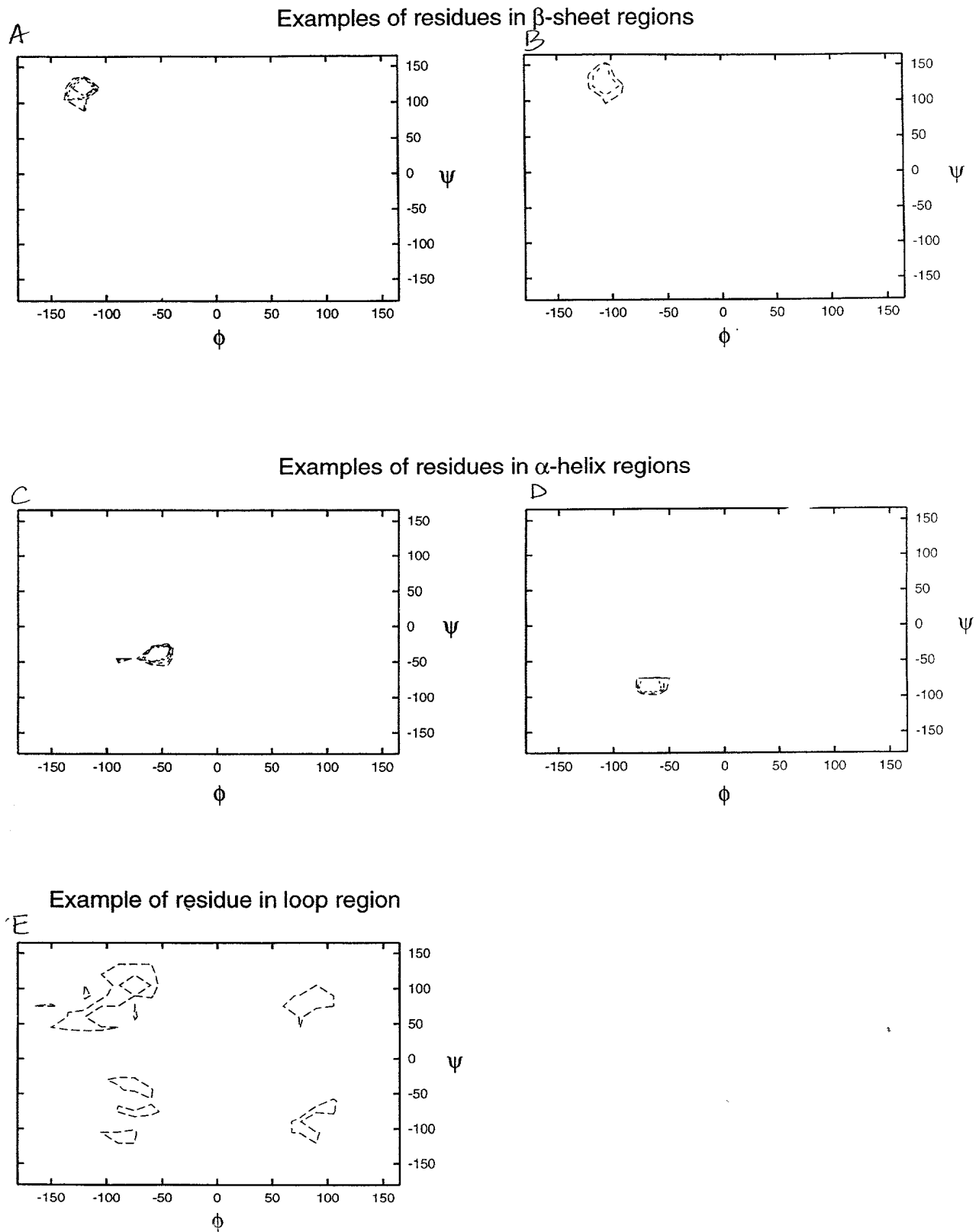


FIGURE 3

FIGURE 4



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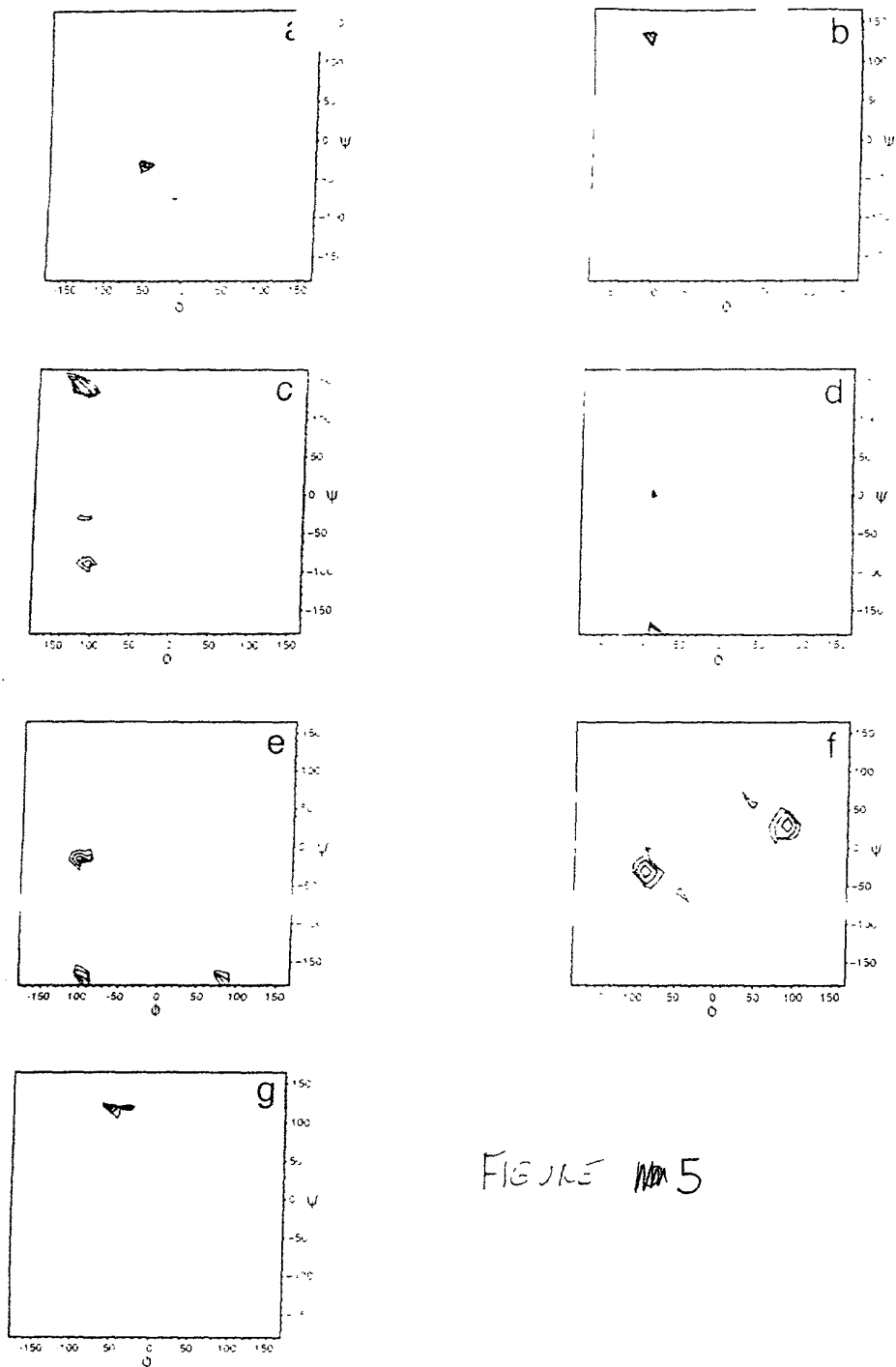
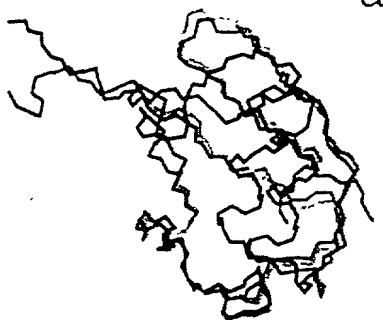
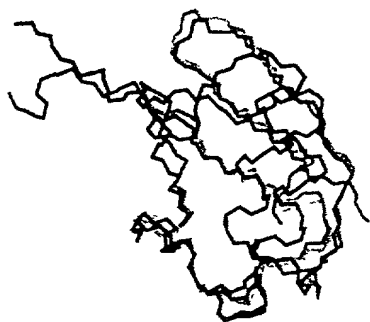
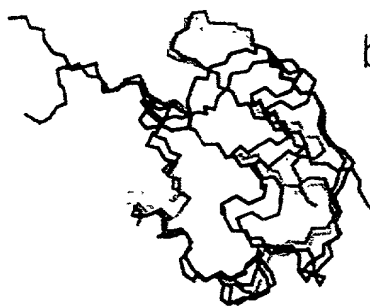


FIGURE 5

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a



b

FIGURE 6

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FIGURE 7

Generate Linear
amino-acid chain

Calculate ϕ, ψ angles
for each peptide pair
using experimental
residual dipolar couplings

Fold Linear sequence
with dihedral angle
and backbone NOE
restraints

Refine structure
using NOE and
dipolar coupling
restraints

FIGURE 7

Dipolar Couplings - Powerful Structural Constraints



$$D \propto (3 \cos^2 \theta - 1) / r^3$$

J + D (Hz)



FIGURE 8

FIGURE 9

Measurement of Dipolar Couplings Requires a Weakly Aligned Molecule

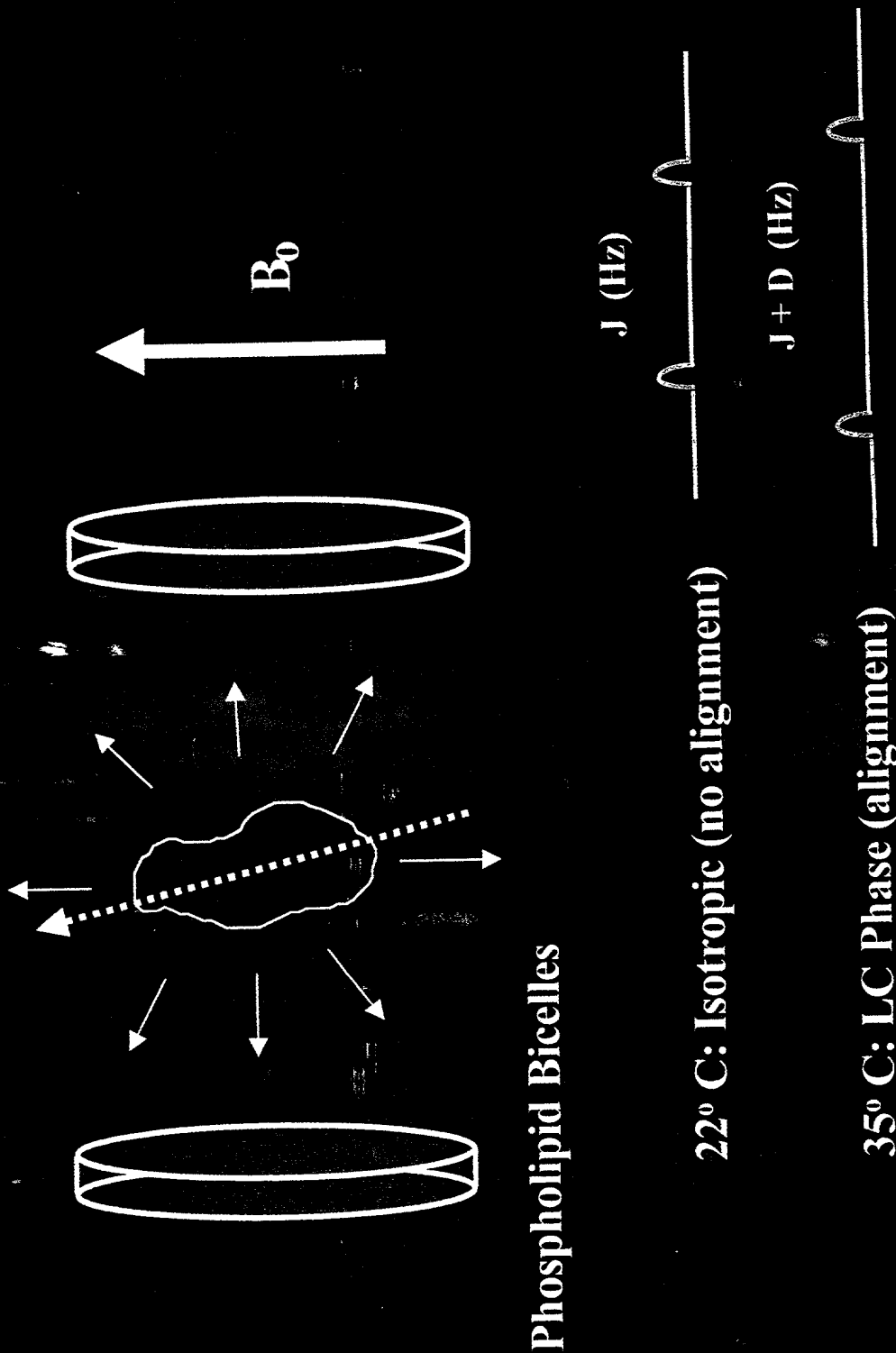
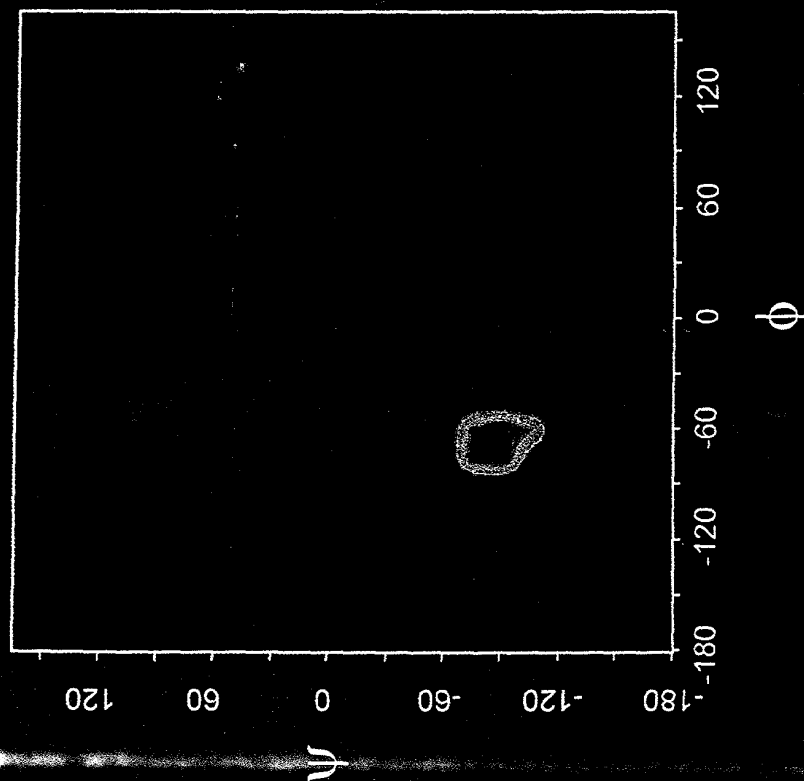


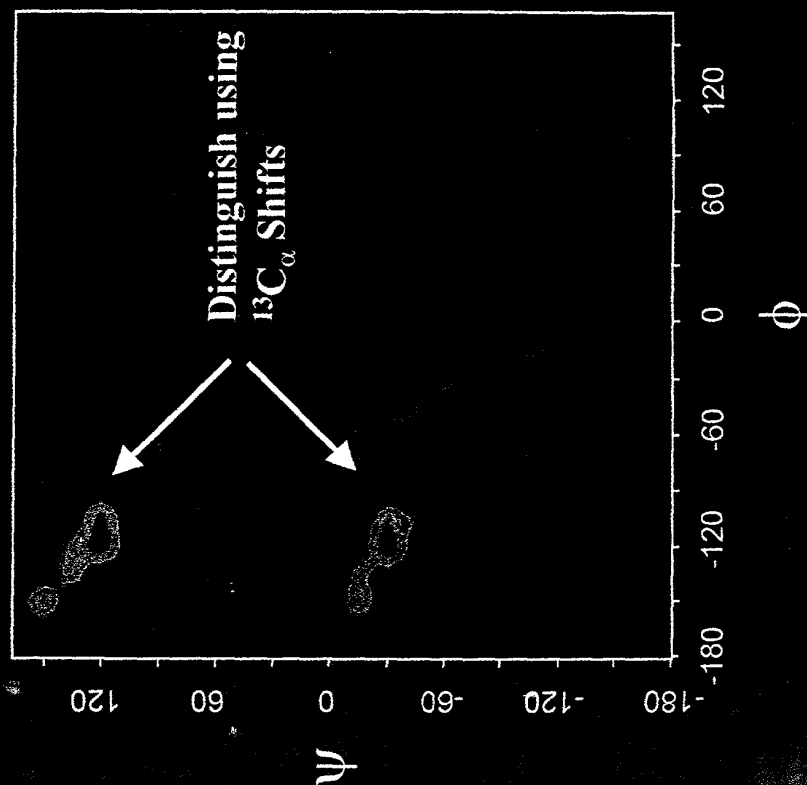
FIGURE 10

ϕ, ψ Mapping Using Residual Dipolar Couplings

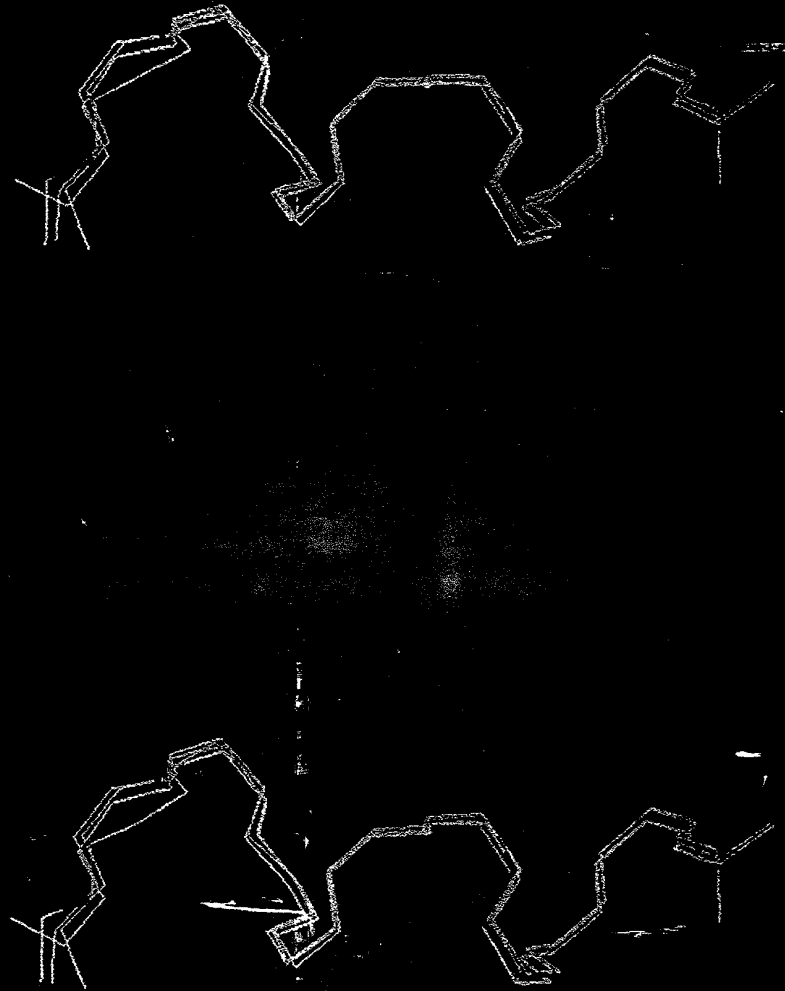
Val 26



Ile 33



NMR vs. Crystal Structure of α -helix (24-34) Ubiquitin



NMR — Crystal

NMR vs. Crystal Structure of β -sheet (3-15) Ubiquitin



NMR — Crystal

FIGURE 12

Crystal Structure vs. NMR Global Fold - Ubiquitin

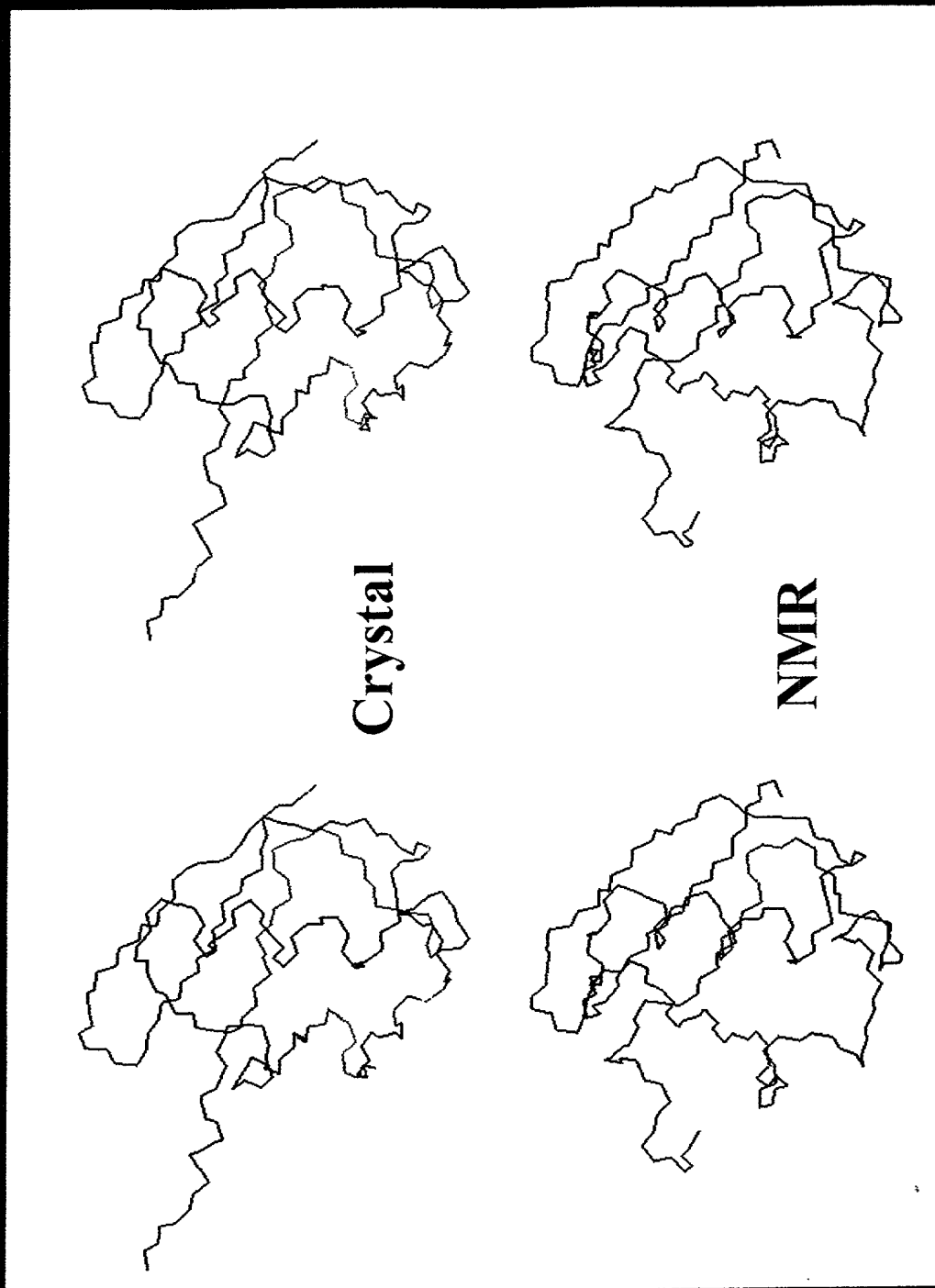


FIGURE 13